A

SYNOPSIS

ON

Studies of magneto-optical transport in tilted multi-Weyl semimetals in the presence of orbital magnetic moment

For the degree of Doctor Of Philosophy in Physics with permission from the department of physics, faculty of Science L.N.M.U, Darbhanga, 846004

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1 Introducton and Review of Literature

Weyl semimetals are a newly discovered class of topological materials with pairs of conduction and valence bands touching at the discrete points in the Brillouin zone (called Weyl points) [1, 2, 3, 4, 5, 6, 7, 8], around which the dispersion relation is linear. This special band structure gives rise to a nontrivial topological property, which can be identified by the Berry curvature that is usually considered as an effective magnetic field in the momentum-space with a monopole located at the Weyl node. According to the Nielsen-Ninomiya theorem [9, 9], the Weyl nodes always appear in pairs, and form a source and sink of this effective field, respectively, which leads to a number of the unusual phenomena, such as high mobility phenomena [10, 11], the existence of Fermi arcs [5, 6, 7, 8], the chiral anomaly [12, 13, 14, 15], and the anomalous Hall effect [16, 17], etc.

The discovery of Weyl semimetals triggers a search for a variety of novel quantum phenomenon. As an important aspect, the magneto-electronic transport properties have been quickly a focus of interest. A series of phenomena related to the chiral anomaly is revealed successively. For example, the negative magnetoresistance has been experimentally observed in Weyl semimetal materials [18, 19, 20, 21, 22]. The planar Hall effect is predicted theoretically in Weyl semimetals, in which a nonzero Hall conductivity has emerged in the plane of the electric and magnetic fields [23]. Additionally, the anomalous Nernst effect has been studied both theoretically and experimentally [24, 25, 26, 27].

Recently, much attention has been paid to the research of the nonlinear magneto-optical responses in the Weyl semimetal materials. In the absence of external mag- netic fields, the second-order optical response in the Weyl semimetals involves injection, shift, and anomalous current.

Interestingly, all these quantities relate to the topological effect of Weyl semimetals, and require breaking inversion symmetry. The injection current is proportional to the Berry curvature and the difference of the velocities of electrons between the conduction band and valence band in Weyl semimetals [28, 29, 30, 31]. The shift current stems from a combined effect of the linear photoabsorption and the shift vector (defined by Berry connections) [29, 32, 33], and has been confirmed by observing a strong second harmonic

Ponchlal Prabhakar
13/04/2024

10/04/2024

signal in TaAs [34]. The nonlinear anomalous current (nonlinear Hall effect) arises from the Berry curvature dipole [35, 36, 37], and has been observed in the materials WTe_2 and Cd_3As_2 [38, 39]. Under the weak magnetic field, the optical activity and the chiral anomaly will contribute to the second-order nonlinear optical response in the Weyl semimetal [40, 41, 42, 43]. Whereas in a strong magnetic field, the third-order responses have an extremely high optical susceptibility originating from the linear energy dispersion near the Weyl nodes [44].

It is known that the "self-rotation" of the Bloch wave packet will induce an orbital magnetic moment [45], and modify the energy of the electron under the external magnetic field, which will change the magneto-optical responses of tilted Weyl semimetals, an issue which is addressed here.

2 Objective of proposed work

In this research proposal, we study the linear and nonlinear magneto-optical responses for tilted Weyl semimetals, where an orbital magnetic moment is introduced. We derive an analytic expression for the magnetoconductivity by means of the Boltzmann equation method. It is found that the orbital magnetic moment induces a new magnetoconductivity term, which gives rise to a partial cancellation for the total magnetoconductivity. This suppressed feature is further manifested by analyzing the linear (B-linear) and quadratic (quadratic-B) contribution in the magnetic field to magnetoconductivities. We also show that no matter in the linear or nonlinear response regime, the B-linear (quadratic-B) magnetoconductivity exhibits a behavior that is dependent (independent) of the chirality of the Weyl node. By incorporating the orbital magnetic moment, we generalize the magneto-optical transport of multi-Weyl semimetals(mWSMs) within a semiclassical approximation. In the linear or nonlinear response regime, an analytic expression for the magnetoconductivity is obtained in the case of single WSMSs, where a new term due to the orbital magnetic moment is added, and leads to a partial cancellation for the total magnetoconductivities in the single WSMs. This suppressed feature has manifested by analyzing the linear and quadratic contribution in the magnetic field to magnetoconductivities. This magnetic orbital moments may be incorporated to study helicons modes in mult-WSMs in further part

Panchlal Prabhat
13/09/2024

13/09/2024

of this research works.

3 Plan of work and Methodology

The non-interacting low energy effective Hamiltonian for tilted multi-Weyl semimetals is given by [46, 47, 48, 49],

$$\mathcal{H}_J = \hbar v_t k_z 1_{2\times 2} + \alpha_J \hbar[(\hat{k}_-)^J \sigma_+ + (\hat{k}_+)^J \sigma_-] + \chi \hbar v_z \hat{k}_z \sigma_z + \hbar v_F t_s k_z \sigma_0, \quad (1)$$

where $\sigma_\pm = \frac{1}{2}(\sigma_x \pm i\sigma_y)$ and $\hat{k}_\pm = \hat{k}_x \pm i\hat{k}_y$, J represents monopole charge, v_z is the effective velocity along $\hat{z}$ direction and α_J is the material dependent parameter, e.g. α_1 and α_2 are the Fermi velocity and inverse of the mass respectively for the isotropic and double WSMs. We will use semiclassical Boltzmann equations and chiral kinetic theory for above our proposed works. Let us briefly outline the both techniques.

For a given chirality $g = \pm$ of a single Weyl node, the semiclassical Boltzmann equation (SBE) reads as follows

$$\frac{\partial \tilde{f}^s}{\partial t} + \dot{k}.\frac{\partial \tilde{f}^s}{\partial k} = \frac{\tilde{f}^s - \tilde{f}^s_0}{\tau} \quad (2)$$

Here, $\tilde{f}^s(\tilde{\epsilon}^s_k)$ is the electron distribution function. where τ is the relaxation time originating from the scattering of electrons by phonons, impurities, electrons, and other lattice imperfections [50]. In the presence of a static magnetic field $\boldsymbol{B}$ and a time varying electric field $\boldsymbol{E}$, the semiclassical equations of motion are [16]

$$\dot{r} = v_g(k) - \dot{k} \times \Omega_g(k) \quad (3)$$

$$\hbar\dot{k} = -eE - e\dot{r} \times B \quad (4)$$

The first term on the right-hand side of Eq. (3) is $v_g(k) = \frac{1}{\hbar}\nabla_p \epsilon_g(k)$,defined in terms of an effective band dispersion $\epsilon_g(k)$. In topological metals such as WSMs, this quantity acquires a term due to the intrinsic orbital moment [16],i.e., $\tilde{\epsilon}^s_k = \epsilon^s_k - m^s_k \cdot B$, while $m_g(p)$ is the orbital moment [16] induced by

Panchlal Prabhat
13/04/2024

Amrit
13/04/2024

the semiclassical "self-rotation" of the Bloch wave packet. The energy dispersion is given by $\epsilon_k^s = \hbar v_t k_z + s\hbar\sqrt{\alpha_n^2(\rho_J)^2 + (k_z v_z)^2}$ with $\rho_J = (k_x^2 + k_y^2)^{J/2}$.

$$\begin{aligned} \Omega_g(\boldsymbol{k}) &= Im[\langle \nabla_k u_k^s| \times |\nabla_k u_k^s\rangle] \\ \boldsymbol{m}_g(k) &= -\frac{e}{2\hbar} Im[\langle \nabla_k u_k^s| \times (\mathcal{H}_J(\boldsymbol{k}) - \epsilon_k^s)|\nabla_k u_k^s\rangle] \end{aligned} \tag{5}$$

where $|u_k^s\rangle$ satisfies the equation $\mathcal{H}_J(\boldsymbol{k})|u_k^s\rangle = \epsilon_k^s|u_k^s\rangle$

$$\begin{aligned} \dot{\boldsymbol{r}} &= \frac{1}{\hbar D}[\boldsymbol{v}_g(k) + e\boldsymbol{E} \times \Omega_g(\boldsymbol{k}) + \frac{e}{\hbar}(\boldsymbol{v}_g(k) \cdot \Omega_g(\boldsymbol{k})\boldsymbol{B}] \\ \hbar\dot{\boldsymbol{k}} &= \frac{1}{\hbar D}[-e\boldsymbol{E} - \frac{e}{\hbar}\boldsymbol{v}_g(k) \times \boldsymbol{B} - \frac{e^2}{\hbar}(\boldsymbol{E}.\boldsymbol{B})\Omega_g(\boldsymbol{k})] \end{aligned} \tag{6}$$

where the factor $D = 1 + \frac{e}{\hbar}(\Omega_g(\boldsymbol{k}) \cdot \boldsymbol{B})$ modifies the phase space volume. Here, γ is a dimensionless control parameter and $\Omega_s(\boldsymbol{k})^{\pm} = \pm\frac{s}{2}\frac{nv\alpha_n^2 k_\perp^{2n-2}}{\beta_{k,s}^3}\{k_x, k_y, nk_z\}$ is the WSM Berry curvature and $\boldsymbol{m}_{k,s}^{\pm} = \frac{s}{2}\frac{env\alpha_n^2 k_\perp^{2n-2}}{\hbar\beta_{k,s}^2}\{k_x, k_y, nk_z\}$ is orbital magnetic moment of multi-WSMs [51].

$$\begin{aligned} \tilde{f}_0^s(\tilde{\epsilon_k^s}) &= \tilde{f}_0^s(\epsilon_k^s - \boldsymbol{m}_k^s \cdot \boldsymbol{B}) \\ &\simeq \tilde{f}_0^s(\epsilon_k^s) - \boldsymbol{m}_k^s \cdot \boldsymbol{B}\frac{\partial \tilde{f}_0^s(\epsilon_k^s)}{\partial \epsilon_k^s} \end{aligned} \tag{7}$$

where $\tilde{f}_0^s(\epsilon_k^s) = 1/[\exp^{(\epsilon_k^s - \mu)/k_B T} + 1]$ with k_B the Boltzmann constant, T the temperature, and μ the chemical potential.

$$\tilde{f}^s = \tilde{f}_0^s + \tilde{f}_1^s \exp^{-i\omega t} + \tilde{f}_2^s \exp^{-2i\omega t} + ... \tag{8}$$

where $\tilde{f}_1^s$ and $\tilde{f}_2^s$ are the first- and second-order terms for $\boldsymbol{E}$, respectively. The electric current density can be calculated by

$$j = -\frac{e}{(2\pi)^3}\int d^3k D\dot{\boldsymbol{r}}\tilde{f}^s \tag{9}$$

From the above formulations, we would calculate both linear and nonlinear longtudinal as well as Hall conductivties. We could also generalize this formulatons for helicons modes of multi-WSMs in second part of this

Panchlal Prabhat
13/04/2024

13/04/2024

research proposal , We will evaluate the optical conductivity of a 3D Weyl semimetal from semiclassical Boltzmann transport theory, with the inclusion of the orbital moment $m_g(p)$ and anisotropic contributions to the distribution function.

4 Expected Results

We would calculate a systematic investigation of the linear and nonlinear magneto-optical responses in tilted Weyl semimetals, derive an analytic expression for the magnetoconductivity by using the Boltzmann equation method, and find that: (i) In the linear response regime, there is a Drude-type conductivity from each Weyl node. In the absence of a magnetic field, the optical conductivity is sensitive to the tilt owing to the anisotropy of the drift velocities in the Weyl semimetals. When the magnetic field is applied, in the tilted Weyl node, the B-linear conductivity consists of two contributions, one from the Berry curvature and the other from the orbital magnetic moment. These two contributions would partly cancel each other, leading to the suppression of the total conductivities in non-trivial ways. (ii) In the second-order nonlinear response regime, without a magnetic field, an analytical formula for the second harmonic conductivity will be derived, showing chirality independence. In the presence of the magnetic field, the B-linear second harmonic conductivities in a single Weyl cone neither vanish nor rely on the tilt. But the diagonal conductivities from two Weyl nodes with opposite chirality cancel each other, while the off-diagonal (Hall) conductivities would also be derived, where these two contributions of Berry-curvature and orbital magnetic moment could be partly cancelled out.

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Amrit 13.9.24

Panchal Prakhar
13/09/2024

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13/04/2024

Panchlal Prakshat
13/04/2024

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13/09/2024

13/9/2024

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Panchal Prabhat
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13/04/2024

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